REPORT DOCUMENTATION PAGE

Form Approved OMB NO. 0704-0188

The public reporting burden for this collection of information is estimated to average 1 hour per response, including the time for reviewing instructions, searching existing data sources, gathering and maintaining the data needed, and completing and reviewing the collection of information. Send comments regarding this burden estimate or any other aspect of this collection of information, including suggesstions for reducing this burden, to Washington Headquarters Services, Directorate for Information Operations and Reports, 1215 Jefferson Davis Highway, Suite 1204, Arlington VA, 22202-4302. Respondents should be aware that notwithstanding any other provision of law, no person shall be subject to any oenalty for failing to comply with a collection of information if it does not display a currently valid OMB control number.
PLEASE DO NOT RETURN YOUR FORM TO THE ABOVE ADDRESS.

1. REPORT DATE (DD-MM-YYYY)	2. REPORT TYPE	3. DATES COVERED (From - To)
05-09-2012	Final Report	15-Jul-2007 - 14-Jul-2012

4. TITLE AND SUBTITLE	5a. CONTRACT NUMBER
Multi-scale and Multi-physics Numerical Methods For Modeling Transport in Mesoscopic Systems	W911NF-07-1-0492
	5b. GRANT NUMBER
	5c. PROGRAM ELEMENT NUMBER
	611102

6. AUTHORS	5d. PROJECT NUMBER
Wei Cai	
	5e. TASK NUMBER
	5f. WORK UNIT NUMBER

7. PERFORMING ORGANIZATION NAMES AND ADDRESSES	8. PERFORMING ORGANIZATION REPORT NUMBER
University of North Carolina - Charlotte Office of Sponsored Programs 9201 University City Blvd. Charlotte, NC 28223 -0001	

9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES)	10. SPONSOR/MONITOR'S ACRONYM(S)
U.S. Army Research Office P.O. Box 12211 Research Triangle Park, NC 27709-2211	ARO
	11. SPONSOR/MONITOR'S REPORT NUMBER(S)
	51057-MA.4

12. DISTRIBUTION AVAILIBILITY STATEMENT

Approved for Public Release; Distribution Unlimited

13. SUPPLEMENTARY NOTES

The views, opinions and/or findings contained in this report are those of the author(s) and should not contrued as an official Department of the Army position, policy or decision, unless so designated by other documentation.

14. ABSTRACT

During this project, we have conducted development of numerical methods for various quantum mechanics models. Accomplishments have been made in the following areas: [1] Adaptive Cell-Average Spectral Element Method for Time Dependent Wigner Equations, [2] Effect of Boundary treatment on transport current in nano-MOSFETs. [3] Accuracy of Frensley inflow boundary conditions.

15. SUBJECT TERMS

quantum transport, nano-devices

16. SECURITY CLASSIFICATION OF:			17. LIMITATION OF ABSTRACT	15. NUMBER OF PAGES	19a. NAME OF RESPONSIBLE PERSON
a. REPORT	b. ABSTRACT	c. THIS PAGE	UU		Wei Cai
UU	UU	UU			19b. TELEPHONE NUMBER
					704-687-4581

Multi-scale and Multi-physics Numerical Methods For Modeling Transport in Mesoscopic Systems

ABSTRACT

During this project, we have conducted development of numerical methods for various quantum mechanics models. Accomplishments have been made in the following areas: [1] Adaptive Cell-Average Spectral Element Method for Time Dependent Wigner Equations, [2] Effect of Boundary treatment on transport current in nano-MOSFETs. [3] Accuracy of Frensley inflow boundary conditions.

Three journal publications have resulted from this effort.

Enter List of papers submitted or published that acknowledge ARO support from the start of the project to the date of this printing. List the papers, including journal references, in the following categories:

(a) Papers published in peer-reviewed journals (N/A for none)

Received	Paper
2011/08/26 1· 2	Sihong Shao, Tiao Lu, Wei Cai. Adaptive Conservative Cell Average Spectral Element Methods for Transient Wigner Equation in Quantum Transport, COMMUNICATIONS IN COMPUTATIONAL PHYSICS, (3 2010): 0. doi: 10.4208/cicp.080509.310310s
2011/08/26 1· 1	Wei Cai, Haiyan Jiang. Effect of boundary treatments on quantum transport current in the Green's function and Wigner distribution methods for a nano-scale DG-MOSFET, Journal of Computational Physics, (06 2010): 0. doi: 10.1016/j.jcp.2010.02.008
2011/08/26 1· 3	Haiyan Jiang, Wei Cai, Raphael Tsu. Accuracy of the Frensley inflow boundary condition for Wigner equations in simulating resonant tunneling diodes, Journal of Computational Physics, (03 2011): 0. doi: 10.1016/j.jcp.2010.12.002

TOTAL: 3

Number of Papers published in peer-reviewed journals:

(b) Papers published in non-peer-reviewed journals (N/A for none)

Received	Paper

TOTAL:

Number of Papers published in non peer-reviewed journals:

(c) Presentations

Number of Presentations: 0.00

Non Peer-Reviewed Conference Proceeding publications (other than abstracts):

Received	Paper

TOTAL:

Number of Non Peer-Reviewed Conference Proceeding publications (other than abstracts):

Peer-Reviewed Conference Proceeding publications (other than abstracts):

Received   Paper

   TOTAL:

Number of Peer-Reviewed Conference Proceeding publications (other than abstracts):

(d) Manuscripts

Received   Paper

   TOTAL:

Number of Manuscripts:

Books

Received   Paper

   TOTAL:

Patents Submitted

Patents Awarded

Awards

Graduate Students

NAME	PERCENT_SUPPORTED
FTE Equivalent:	
Total Number:	

Names of Post Doctorates

NAME	PERCENT_SUPPORTED
Haiyan Jiang	1.00
Steve Xin	0.25
Tiao Lu	0.25
FTE Equivalent:	**1.50**
Total Number:	**3**

Names of Faculty Supported

NAME	PERCENT_SUPPORTED	National Academy Member
Wei Cai	0.25	
FTE Equivalent:	**0.25**	
Total Number:	**1**	

Names of Under Graduate students supported

NAME	PERCENT_SUPPORTED
FTE Equivalent:	
Total Number:	

Student Metrics
This section only applies to graduating undergraduates supported by this agreement in this reporting period

The number of undergraduates funded by this agreement who graduated during this period: 0.00

The number of undergraduates funded by this agreement who graduated during this period with a degree in science, mathematics, engineering, or technology fields:...... 0.00

The number of undergraduates funded by your agreement who graduated during this period and will continue to pursue a graduate or Ph.D. degree in science, mathematics, engineering, or technology fields:...... 0.00

Number of graduating undergraduates who achieved a 3.5 GPA to 4.0 (4.0 max scale):...... 0.00

Number of graduating undergraduates funded by a DoD funded Center of Excellence grant for Education, Research and Engineering:...... 0.00

The number of undergraduates funded by your agreement who graduated during this period and intend to work for the Department of Defense 0.00

The number of undergraduates funded by your agreement who graduated during this period and will receive scholarships or fellowships for further studies in science, mathematics, engineering or technology fields:...... 0.00

Names of Personnel receiving masters degrees

NAME
Total Number:

Names of personnel receiving PHDs

NAME
Total Number:

Names of other research staff

NAME	PERCENT_SUPPORTED
FTE Equivalent:	
Total Number:	

Sub Contractors (DD882)

Inventions (DD882)

Scientific Progress

***Statement of the problem:

Due to the quantum nature of the electron transport in nanoscale devices, quantum transport models including Wigner equations and Non-equiblibrium Green's functions are required to compute the current in those devices. Our main goal is to develop accurate and efficient numerical algorithms to compute these quantum transport models.

***Summary of Results:

We have made scientific progress in the following three areas of accomplishments:

In paper [1] on Conservative Adaptive Cell-Average Spectral Element Method for Time Dependent Wigner Equations. We designed and tested a new conservative adaptive spectral element method using cell-average formulation for the time dependent Wigner equations for non-equilibrium transport. The main challenge in this approach is the cost associated with the high dimensional problem in phase space variables (6 for 3-D device in addition to the time variable). To reduce this cost, we propose a Cell-Average representation of the Wigner distribution function $f(x; k; t)$ in the k-space, which allows exact enforcement of conservation of electron mass and adaptive meshing in the phase space using domain decomposition technique.

In paper [2] on effect of treatment of quantum device boundary on the transport current: A nano-scale Double gate MOSFET is investigated with both nonequilibrium Green's function (NEGF) and Wigner distribution methods,each with different treatment of the device boundaries. The NEGF handles the device-contact condition through a self energy term while the Wigner distribution function method employs inflow flux conditions using the Fermi-Dirac electron distribution inside the contact. Numerical results have shown higher transport current at a given gate voltage with the Wigner distribution approach. As the current-voltage (I-V curve) characteristic is the key measurement of a quantum device, correct current simulation will be important in quantum device modeling.

In paper [3] on Accuracy of Frensley inflow boundary conditions: Continuing the studies in [2] above, We carefully investigate the accuracy of the Frensley inflow boundary
condition of the Wigner equation in computing the I-V characteristics of a Resonant Tunneling Diode (RTD). We found that the Frensley inflow boundary condition for incoming electrons holds only exactly infinite away from the active device region and its accuracy depends on the length of contacts included in the simulation. For this study, the non-equilibrium Green's function (NEGF) with a Dirichlet to Neumann mapping boundary condition is used for comparison. The I-V characteristics of the RTD are found to agree between self-consistent NEGF and Wigner methods at low biaspotentials only with sufficiently large GaAs contact lengths.

*** Bibliography

[1] Sihong Shao, Tiao Lu, Wei Cai. Adaptive Conservative Cell Average Spectral Element Methods for Transient Wigner Equation in Quantum Transport, COMMUNICATIONS IN COMPUTATIONAL PHYSICS, (3 2010): 0. doi: 10.4208/cicp.080509.310310s

[2] Wei Cai, Haiyan Jiang. Effect of boundary treatments on quantum transport current in the Green's function and Wigner distribution methods for a nano-scale DG-MOSFET, Journal of Computational Physics, (06 2010): 0. doi: 10.1016/j.jcp.2010.02.008

[3] Haiyan Jiang, Wei Cai, Raphael Tsu. Accuracy of the Frensley inflow boundary condition for Wigner equations in simulating resonant tunneling diodes, Journal of Computational Physics, (03 2011): 0. doi: 10.1016/j.jcp.2010.12.002

Technology Transfer